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The *d*-Electron Entropy in the Wills-Harrison Approximation with Non-Diagonal Couplings between *d* Electrons

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Abstract

It is shown that the full account of the non-diagonal couplings between *d* electrons sited on different atoms in a transition metal implemented within the framework of the Wills-Harrison model leads to vanishing the *d*-band contribution to the entropy.

Keywords: Entropy, transition metal, Wills-Harrison model, *d*-state coupling

The electron contribution to the entropy of a metal is expressed as follows (hereafter, in atomic units per atom):

$$S_e = (\pi k_B)^2 T n(\varepsilon_F)/3 \quad , \tag{1}$$

where ε_F is the Fermi energy, k_B - Boltzmann constant, T - absolute temperature $n(\varepsilon)$ - full electron density of states:

$$n(\varepsilon) = n_d(\varepsilon) + \sqrt{\varepsilon}/(2\pi^2\rho) \quad , \tag{2}$$

where $n_d(\varepsilon)$ is the density of the *d*-electron states, ρ - mean atomic density.

Different approximations can be used for description of $n_d(\varepsilon)$. In particular, Wills and Harrison (WH) [1] used the rectangular approximation [2]. In [3] the Lorenz form of $n_d(\varepsilon)$ was used:

$$n_d(\varepsilon) = \frac{10W}{\pi[(\varepsilon - \varepsilon_F + W/\tan(\pi z_d/10))^2 + W^2]}, \quad (3)$$

where W is the *d*-band width, z_d - effective *d*-electron valence.

As was shown in [4], the full account of the non-diagonal couplings between *d* electrons sited on different atoms in a transition metal implemented within the framework of the Wills-Harrison model [5] leads to vanishing the *d*-band contribution to the internal energy due to vanishing the *d*-band width.

Since within any approximation $n_d(\varepsilon) = 0$ at $W = 0$, the same conclusion can be made for the *d*-band contribution to the entropy.

In conjunction with the results [4, 6] it denotes that no the *d*-electron-depended terms in the free energy of a transition metal in the case of the full account of the non-diagonal couplings between *d* electrons.

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